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Graph-based Framework for 3-D Vascular Dynamics Simulation

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Abstract

Vascular network dynamics has crucial impact on vertebrate physiology and numerous diseases are indicated by its malfunctioning. As a consequence, there is a high demand for tools facilitating the studies of the associated phenomena. However, many of them are focused strictly on the 2-D environments, similar to the ones used by *in vitro* research. Hence, they are rather useless for tumour development or drug interactions modelling purposes, as those processes need to be investigated in a 3-D setup. We address this issue by proposing a novel framework that allows to simulate vasculature growth and restructuration in 3 dimensions. Our solution yields morphologically accurate results, exhibiting properties found in real-world data, such as vein-artery interdigitation. Its graph-based architecture streamlines the outcome analysis and enables a straightforward way of including additional workflow extensions.

Keywords: mathematical modelling, pattern evolution, vascular system dynamics, complex networks

1 Introduction

Vascular growth and remodelling is an active process that affects blood vessels spatial structure by ongoing cell growth, death and migration. It is a total effect of work performed by three major mechanisms: vasculogenesis (capillary formation from progenitor cells), angiogenesis (budding of new branches from the pre-existing vessels), and arteriogenesis (increase of the vessel luminal diameter in response to the increased blood flow). The resulting circulatory system organisation has a crucial impact on living organisms evolution, development, and pathophysiology. Majority of human mortal diseases (including cancer) is hallmarked by changes in tissue vascularization [1]. The studies on its influence on tumour aggressiveness have shown that heterogeneous network promotes a higher amount of cellular turnover, which is characteristic for the more dangerous tumour classes [2].

Enhancing our understanding of phenomena that govern vessel proliferation and regression is mandatory in order to formulate more effective treatment of numerous angiogenesis-dependent

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ailment states. As a consequence, vessel network dynamics continue to be a relevant research area, engaging professionals from various field of science, as diverse as medicine or mathematics [3].

A standard approach to conducting those studies is by carrying out a series of experiments utilising either an *in vivo* (such as chick chorioallantoic membrane, zebrafish or rat sponge implants) or *in vitro* (mostly based on human endothelial cells) models. The main reason for doing so is the desire to capture complex interactions that are present in the underlying biological system but may be absent when using a more simplified representation [4].

However, there are certain drawbacks associated with the aforesaid techniques. They are expensive, time consuming, and it is often hard to reproduce them faithfully. Furthermore, the obtained outcomes are frequently undermined by problems with data acquisition and with choosing the right evaluation assays. When said issues are combined with the trial and error strategy (typical for early stages of investigation process) the efficiency of involved researchers is substantially hindered. Therefore, it is hardly surprising that alternative methods employing computing technologies (customarily called *in silico*), which allow to execute vast numbers of examinations at any level of detail repeatedly and in controlled manner, are constantly becoming more and more popular [5][6][7][8].

A wide range of simulational models depicting vascular network evolution were developed through the years, concentrating on different aspects of the portrayed phenomenon and operating on various spatial and temporal scales. Wcisło et al. employed complex automata combined with particle dynamics to include angiogenic processes in their multiscale model of tumour progression [9]. Parsonson utilised MicroCT scans to provide credible initial conditions for the later growth [10]. Lee et al. examined the way in which vasculature transforms into its highly inhomogeneous tumour specific morphology [11]. Other studies explored the response to drug application [12], focused on anastomosing vessels [13] or attempted to track individual cells [14].

Complex network dynamics are another field of research that emerged recently and gained a lot of attention, as it struggles to formulate universal laws applicable to graph-like being appearing in all sciences [15]. Among them vascular graphs are an unusual and curious family, as they do not necessary exhibit traits that are commonly found in other vigorously studied ones, such as the small world property typical for the social graphs. Unfortunately, attempts at studying them are obstructed by restricted access to high quality datasets, as the information about blood vessel connection structure needs to be extracted from available medical images (angiograms), which tend to be scarce and hard to process or result in relatively small and mundane samples [16].

Thus, the computational models that are able to efficiently generate large, nontrivial vasculatures and offer flexible configuration of initial geometry and conditions are especially valued by scientists engaging in network exploration. A well-received one that meets the mentioned was proposed by Gödde and Kurz in [17] and allows to simulate microvascular growth and remodelling into arteries and veins. Nevertheless, it has one serious deficiency — being limited to the two-dimensional space only. The aim of this work is to extend that model, find its generalization capable of functioning in three dimensions, and in consequence cover a wider range of applications.

2 Proposed Framework

The basic workflow of the proposed framework is outlined in Fig. 1 as a UML activity diagram. It starts by loading the initial conditions and filling the environment with randomly generated graph. Then based on its structure the pressure potential field (and the derived properties)